

Non-equilibrium dynamics of the driven Hubbard model.

A. Amaricci^{1,3}, C. Weber², M. Capone^{1,3}, G. Kotliar⁴

¹ *CNR-IOM, SISSA, Via Bonomea 265, 34136 Trieste, Italy.*

² *Cavendish Laboratory, Cambridge University, J.J. Thomson Ave., Cambridge, UK*

³ *Physics Department, University "Sapienza", Piazzale A. Moro 2, 00185 Rome, Italy. and*

⁴ *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*

(Dated: February 2, 2012)

We investigate the dynamics of a two-dimensional Hubbard model in a static electric field in order to identify the conditions to reach a non-equilibrium stationary state. For a generic electric field, the convergence to a stationary state requires the coupling to a thermostating bath absorbing the work done by the external force. Following the real-time dynamics of the system, we show that a non-equilibrium stationary state is reached for essentially any value of the coupling to the bath. We map out a phase diagram in terms of dissipation and electric field strengths and identify the dissipation values in which steady current is largest for a given field.

PACS numbers: 71.10.Fd, 05.70.Ln, 05.30.Fk

The theoretical investigation of out-of-equilibrium strongly correlated quantum systems recently generated tremendous interest, stimulated by novel experimental techniques which allow to explore transport properties of correlated materials in a non-equilibrium regime, notwithstanding the recent achievements in the field of optically trapped cold-atoms. These experimental advances posed serious challenges to the theory, which require the development of new ideas to be tackled. In fact, although we achieved a fair understanding of correlated materials at equilibrium, we are just beginning to uncover the basic principles governing quantum systems far from equilibrium.

Dynamical mean-field theory (DMFT) is an established method to investigate correlated materials [1]. The recent extension of the DMFT out of equilibrium [2, 3], provides us with a reliable tool to clarify how correlation effects influence the non-equilibrium dynamics of quantum systems. Non-equilibrium DMFT has been successfully applied to study quantum quenches - sudden changes of some control parameter[4], and to investigate driven correlated systems[2, 5]. In this context, DMFT has been used to show how interactions favor the formation of stationary states by suppressing Bloch oscillations of the current[2, 5, 6] and to analyze the dielectric breakdown of Mott insulators[7].

In this work we focus on the role of the coupling to an external thermostat in the out-of-equilibrium dynamics of a correlated system and we show when and how it leads to a non-equilibrium stationary state (NSS). Despite its importance, the role of dissipation in driven correlated systems has only been discussed assuming the existence of a NSS[8], while we are not aware of any study following the real-time dynamics leading to such state. In the classical framework, dissipation is usually introduced by coupling the system to a set of reservoirs that ultimately impose a suitable constraint on the equations of motion[9]. Nevertheless, the direct extension of this approach to the

quantum regime is not straightforward because of the Hamiltonian nature of the quantum equations[10].

To include dissipation effects we couple the Hubbard model, the paradigm of strong correlations, to a fermionic bath. We follow the real-time dynamics when the system is driven out of equilibrium by a static electric field. We show that, for a given value of the electric field, coupling to the thermostat is necessary to reach a physically relevant NSS. Remarkably, a NSS with finite current can be reached for almost any value of the dissipation regardless the initial conditions. The coupling to a bath is therefore also an essentially sufficient condition to dynamically approach the NSS. Finally, we characterize the properties of the NSS in terms of local observables and construct the phase-diagram of the model.

Model. We consider the two-dimensional Hubbard model on a square lattice with spacing a . The model Hamiltonian reads ($c = 1$):

$$\mathcal{H}_c = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k} - e\mathbf{A}(t)) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_i \tilde{n}_{i,\uparrow} \tilde{n}_{i,\downarrow} \quad (1)$$

where $\tilde{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} - 1/2$. This model describes a half-filled band of conduction electrons with dispersion $\varepsilon(\mathbf{k})$ and hopping amplitude $J_h = 1$ (setting the energy unit of the problem) subject to a local Coulomb repulsion of strength U . The system is coupled to a constant and homogeneous electric field \mathbf{E} , derived from a purely vector potential $\mathbf{A}(t) = -r(t)\mathbf{E}t$, with $\mathbf{E} = E\mathbf{Q}$ and $\mathbf{Q} = (\pi, \pi)$. The function $r(t)$ specifies the switching protocol of the field. In this work we consider $r(t) = \theta(t - t_0)$, corresponding to a sudden switch on of the electric field. Different choices for $r(t)$ will be explicitly stated. The electric field unit is eEa . The coupling to electric field is realized via the Peierls substitution: $\mathbf{k} \rightarrow \kappa = \mathbf{k} - e\mathbf{A}(t)$.

In a solid state system the work done by the electric field on the electrons is constantly transformed into heat by various scattering mechanisms. Thus, coupling to an external thermostat is crucial to maintain the internal en-

ergy conserved on average. A thermostating mechanism is realized by assuming the system to be locally coupled to a bath of non-interacting electrons at a temperature $T = 0.01$ and which are unaffected by the electric field. As the details of the internal structure of the thermostating reservoirs are irrelevant with respect to the physics of the NSS, we consider a set of identical systems with constant density of states with a bandwidth W . The coupling has the form:

$$\sum_{\mathbf{k}\sigma} \sum_l V_{\mathbf{k}l} \left(c_{\mathbf{k}\sigma}^\dagger b_{l\sigma} + h.c. \right)$$

For simplicity we choose $V_{\mathbf{k}l} \equiv V$ and we drop any reference to spin index.

The Kadanoff-Baym-Keldysh[11] formalism provides a natural framework to investigate the dynamics in out-of-equilibrium conditions. In the presence of sizeable electric fields the non-equilibrium dynamics is expected to be driven by the field and by the coupling to the thermostat. Being interested in the relaxation towards the NSS, we can simplify the treatment considering only the real-time branches in the Keldysh contour and neglecting the imaginary-time segment. As a consequence, at time t_0 we will simultaneously switch-on the electric field E and the interaction U , introducing also a correlation quench. This is not expected to strongly influence the results in the presence of the thermostat, which is able to dissipate the extra energy involved in the quench as well as the energy pumped by the field [12].

The thermostated system obeys the following Dyson equation on the Keldysh contour \mathcal{C}

$$G_\kappa = \mathcal{G}_{0\kappa} + \mathcal{G}_{0\kappa} \cdot \Sigma_\kappa \cdot G_\kappa \quad (2)$$

where all quantities represent continuous operator of two time variables $(t, t') \in \mathcal{C}$, the symbol \cdot denotes the convolution product $f \cdot g = \int_{\mathcal{C}} dz f(t, z) g(z, t')$ and Σ_κ denotes the Keldysh self-energy function. The non-interacting lattice Green's function $\mathcal{G}_{0\kappa}$ is given by:

$$\begin{aligned} \mathcal{G}_{0\kappa}^{-1}(t, t') &= [G_{0\kappa}^{-1}(t, t') - \Sigma_0(t - t')] \\ G_{0\kappa}^{-1}(t, t') &= [i\vec{\partial}_t - \varepsilon(\kappa)] \cdot \delta_{\mathcal{C}}(t, t') \end{aligned} \quad (3)$$

where $\delta_{\mathcal{C}}$ indicates the delta function on the contour \mathcal{C} , $\Sigma_0(t - t') = V^2 g(t - t')$ and $g(t - t')$ the Fourier transform of the non-interacting local bath Green's function $g(\omega) = [\ln |(W + \omega)/(W - \omega)| - i\pi\theta(W - |\omega|)]/2W$. Thus, the effective coupling to the thermal reservoirs is $\Lambda = V^2/2W$.

Applying $\mathcal{G}_{0\kappa}^{-1}$ on both sides of the Eq. 2 and using Eq. 3, we recast the Dyson equation into the Kadanoff-Baym equation, that is the equation of motion for the Keldysh Green's function, which reads[13]:

$$\begin{aligned} [i\vec{\partial}_t - \varepsilon(\kappa) - \Sigma_0] \cdot G_\kappa^> &= \Sigma_\kappa^R \cdot G_\kappa^> + \Sigma_\kappa^> \cdot G_\kappa^A \\ G_\kappa^< \cdot [-i\vec{\partial}_{t'} - \varepsilon(\kappa) - \Sigma_0] &= G_\kappa^R \cdot \Sigma_\kappa^< + G_\kappa^< \cdot \Sigma_\kappa^A \end{aligned} \quad (4)$$

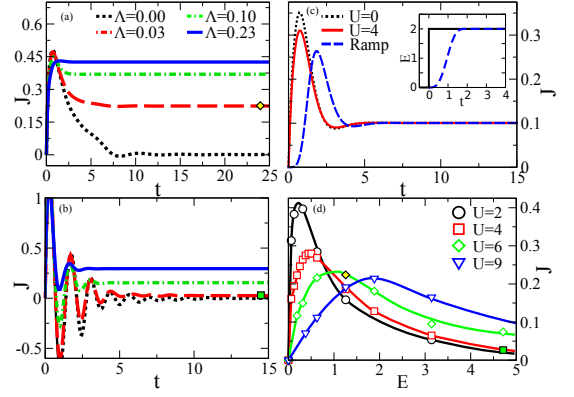


Figure 1. (Color online) (a) dynamics of the local current J for $U = 6$, $E = 1.26$ and increasing coupling to thermostat Λ . (b) same as (a) and $U = 4$ and $E = 4.7$. (c) dynamics of the local current from different realizations of the initial conditions: electric field quench on the non-interacting $U = 0$ (black) and interacting $U = 4$ state (red), smooth switch-on of the electric field for $U = 0$ and $\tau = 2$ (blue) (see text). The inset show the profile of the electric field. (d) linear/non-linear crossover of the steady current as a function of the electric field E . Data for $\Lambda = 0.025$.

As an effect of the symmetries relating the Keldysh components, Eqs. 4 determine a system of coupled ordinary first-order differential equations in the (t, t') -plane for the lattice Keldysh Green's function G_κ . The numerical solution of this system[14] permits to obtain G_κ up to arbitrary large times, once suitable initial conditions are specified. We fixed the time-step parameter, introduced by discretization of the contour \mathcal{C} , to $\delta t < 0.1$. The initial conditions for the system 4 are given specifying the value of momentum distribution at an (arbitrary) initial time $t = t_0$. In this Letter we set $n_{\mathbf{k}}(t_0 = 0) = -iG_{\mathbf{k}}^<(0, 0) = f(\varepsilon(\mathbf{k}))$, with f the Fermi-Dirac distribution, except where otherwise stated.

We use DMFT to deal with correlations in a non-perturbative way. Within DMFT the lattice self-energy is replaced by its local component, so that momentum dependence is determined by the non-interacting dispersion. The self-energy can be derived from the self-consistent solution of an impurity problem written in terms of a local Weiss field \mathcal{G}_0 . This latter describes the effective medium coupled to the impurity and has to be self-consistently determined solving the following equations:

$$\begin{aligned} \mathcal{G}_0^R &= \Gamma \cdot G_{\text{loc}}^R; \quad \Gamma = [\mathbb{I} + G_{\text{loc}}^R \cdot \Sigma^R]^{-1} \\ \mathcal{G}_0^> &= \Gamma \cdot G_{\text{loc}}^> \cdot \Gamma^\dagger + \mathcal{G}_0^R \cdot \Sigma^> \cdot \mathcal{G}_0^{R\dagger} \end{aligned} \quad (5)$$

where local functions are obtained summing the solution of Eqs. 4 for any $\mathbf{k} \in [-\pi, \pi]^2$: $F_{\text{loc}} = \sum_{\mathbf{k}} F_{\mathbf{k}}$. To close the DMFT equations it is necessary to determine the impurity self-energy $\Sigma(t, t')$. In this work we use iterated

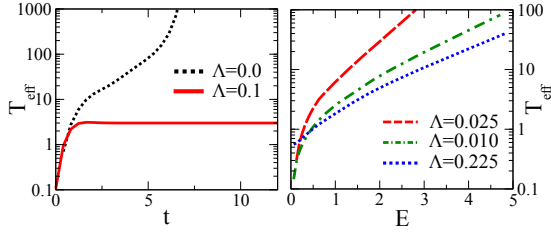


Figure 2. (Color online) Left panel: effective temperature evolution $T_{\text{eff}}(\Omega)$ for $U = 6$, $E = 1.9$. Right panel: effective temperature T_{eff} as a function of the electric field, for $U = 4$ and increasing coupling to thermostat.

second-order perturbation theory in U [1]:

$$\Sigma^{\geq}(t, t') = U^2 [\mathcal{G}_0^{\geq}(t, t')]^2 \mathcal{G}_0^{\leq}(t', t) \quad (6)$$

Equations 4, 5 and 6 are iterated until a self-consistent solution is obtained.

Results. The approach to the stationary non-equilibrium state can be characterized following the real-time dynamics of suitable observables, such as the local current $\mathbf{J}(t) = -ie/\pi \sum_{\kappa} \mathbf{v}_{\kappa} G_{\kappa}^{\leq}(t, t)$, where $\mathbf{v}_{\kappa} = \nabla_{\kappa} \varepsilon(\kappa)$ is the electronic velocity field. We focus on the correlated metallic phase. Our results for the local current are presented in Fig. 1. The application of a constant electric field on a periodic lattice structure produces an oscillating current (Bloch oscillations) of frequency $\omega_B = eEa$. In the absence of coupling to the external bath ($\Lambda = 0$), the electron-electron interactions suppress the Bloch oscillations leading to an exponentially decaying current which eventually converges to zero at very long time [see panels (a)-(b)]. However, the relaxation process shows two different regimes depending on the value of the interaction U as found in [6].

The non-equilibrium dynamics of the system dramatically changes in presence of finite coupling to the thermostat ($\Lambda > 0$). The local current relaxes to a finite value corresponding to the formation of a NSS. This effect is detailed in panels (a)-(b) for two different values of the electric field. The approach to the NSS is found to be independent from the initial conditions, confirming that the non-equilibrium physics is governed by the field and the dissipation term. In panel (c) of Fig. 1 we compare the solutions obtained using initial conditions $r(t) = \theta(t)$ and $n_{\mathbf{k}}(0) = f(\varepsilon(\mathbf{k}))$ with the solutions obtained: (i) starting from the interacting equilibrium momentum distribution for $U = 4$, (ii) using smooth switching of the electric field $r(t) = [1 - 3/2 \cos(\pi t/\tau) + 1/2 \cos(\pi t/\tau)^3]/2$. The convergence to the same NSS is evident.

In panel (d) of Fig. 1 we plot the steady current which shows a linear/nonlinear crossover as a function of the electric field [cf. panel (d)] [15, 16]. At small fields the current is linear in E , as expected by continuity with perturbed equilibrium state, then it reaches a maximum before decreasing as the field is further increased.

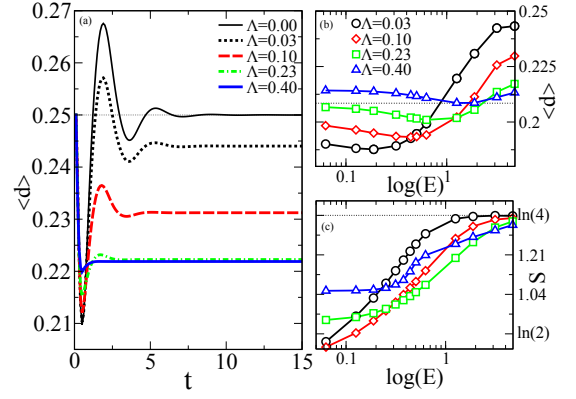


Figure 3. (Color online) (a) Non-equilibrium dynamics of the double occupations $\langle d \rangle$ for $U = 6$, $E = 1.25$ and increasing Λ . (b) Double occupancy of the NSS as a function of the electric field E for $U = 6$. The equilibrium solution for the same value of the interaction (dotted line) is reported for comparison. (c) Entropy S (see text) as a function of the electric field E , for $U = 4$ and the same value of Λ as in (b).

A better understanding of the effects introduced by inclusion of a thermostat is obtained looking at the effective temperature T_{eff} . This is defined as the temperature associated to an equilibrium solution with the same energy $\Omega(t) = \langle K \rangle + \langle V \rangle$ of the non-equilibrium state [6, 7] and the same value of the interaction. For $\Lambda = 0$ the effective temperature rapidly diverges due to the Coulomb scattering between accelerated electrons. In the presence of dissipation the effective temperature relaxes instead to a finite value. The coupling to the thermostat provides a competing scattering channel which prevents the population of high-momentum states and allows the conservation (on average) of the total energy and a constant effective temperature.

In the right panel of Fig. 2 we show the behavior of the effective temperature of the NSS. For any given coupling Λ , T_{eff} is a monotonically increasing function of the electric field, so that arbitrarily large fields imply arbitrarily large T_{eff} . For large fields T_{eff} is depressed by the increasing of the coupling Λ . [However at smaller fields $E < 1$ we observe a non-monotonic behavior of the effective temperature, due the increased scattering with bath degrees of freedom.]

A key quantity to characterize correlated systems is the double occupancy $\langle d \rangle$ which is proportional to the potential energy and measures the effectiveness of correlations. In panel (a) of Fig. 2 we illustrates the formation of NSS from the dynamics of $\langle d \rangle$. In the non-thermostated case ($\Lambda = 0$) $\langle d \rangle$ relaxes to the non-interacting value $\langle d \rangle = 1/4$. Conversely, a finite coupling to the thermostat induces the relaxation to a NSS, which is characterized by a smaller value $\langle d \rangle < 1/4$. The stationary double occupancy, plotted in panel (b) as a function of E , is usually different from the corresponding equilibrium value. Remarkably, the evolution of $\langle d \rangle$ as a function of

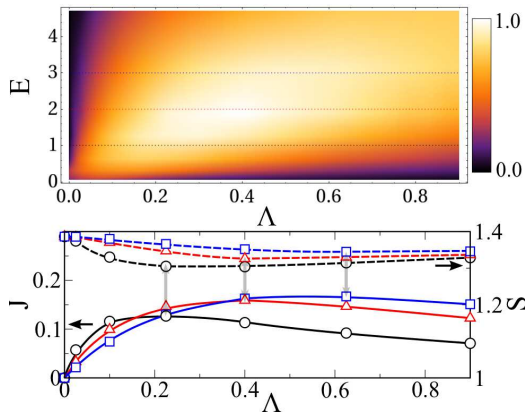


Figure 4. (Color online) Top panel: phase-diagram of the thermostated non-equilibrium Hubbard model. Diagram is obtained from the normalized local current J as a function of electric field strength E and coupling to thermal bath Λ . Horizontal lines indicate the cuts shown in the bottom panel. Bottom panel: local current J and entropy S behavior as a function of Λ , for $E = 1$ (circles), $E = 2$ (triangles), $E = 3$ (squares).

the electric field presents a minimum at a characteristic value of the field strength. This behavior suggests that small applied fields, in conjunction with finite dissipation, increase the degree of electron localization in the NSS. Since the effective temperature of the NSS increases with the electric field, we can connect this result with the Pomeranchuk effect observed in equilibrium. In the latter case the more localized state is favored at finite temperature because of its larger spin entropy[1]. Upon increasing Λ , $\langle d \rangle$ rapidly reduces its range of variation getting closer to the equilibrium value ($\Lambda = E = 0$) for all values of E , implying that, in terms of correlation properties, the NSS becomes closer to the equilibrium state as the dissipation increases.

Further information about the NSS can also be obtained evaluating the function $S = -2 \sum_{\kappa} n_{\kappa} \ln(n_{\kappa})$ which would coincide with the equilibrium entropy at $U = 0$. The extension of entropy for non-equilibrium systems is a debated issue[17] which goes beyond the aim of this paper. Therefore we use S simply as a tool to extract information about the approach to a stationary state and we do not interpret it as a physical entropy. In the absence of a thermostat S dynamically saturates to its high-temperature limit $S = \ln 4$, corresponding to the approach to the zero current stationary state. A substantial reduction of S in the non-linear regime is achieved by coupling the system to the thermostat, as detailed in Fig. 2(c). Nevertheless, for a given coupling Λ , S in the NSS is a monotonically increasing function of the electric field and reaches its limiting value for large enough electric fields, in agreement with the unbounded increase of the effective temperature at constant coupling Λ .

The dependence of the steady current on the coupling

Λ and the electric field can be cast in a diagram in the $(E-\Lambda)$ plane shown in Fig. 4. At the borders of the diagram we identify two small regions where the systems shows small or null steady current. Near the $\Lambda = 0$ axis, the energy injected by the field largely overcomes that absorbed by the thermostat, so that the continuous heating ultimately leads to a reduction of the steady current. Conversely, near the $E = 0$ axis, the large scattering introduced by strong coupling to thermostat reduces the linear conductivity and thus the corresponding steady current. In a wide intermediate region centered around the diagonal of the phase-diagram ($E/2\pi \simeq \Lambda$) we found largest values of the steady current. In this region the dissipation is sufficient to get rid of the extra energy pumped in by the field, but it is not too large to overcome the effect of the field driving a coherent current. The bottom panel shows the current and S along the three horizontal cuts in the diagram, underlining that in the intermediate region the current is maximal and S is minimal.

Conclusions. Using DMFT in combination with a direct solution of the Kadanoff-Baym equations we investigated the non-equilibrium dynamics of the two-dimensional driven Hubbard model coupled to electronic reservoirs. We reported that for a generic value of the field the coupling to an external bath is a necessary and, remarkably, also a sufficient condition to reach a non-stationary steady state with a finite current. We characterized the properties of the NSS in terms of experimentally accessible quantities and studied their dependence on the coupling to the thermostat, identifying the conditions to obtain a maximum of the steady current for a given field. Our work is a fundamental step towards a satisfactory description of non-equilibrium solids, in which a certain degree of dissipation is always present. An explicit coupling to a thermostat is shown to be essential to obtain a description of a non-equilibrium stationary states with finite effective temperature, in contrast to a modelling which neglects dissipation effects and that can only give rise to transient states whose relevance for the physics of actual materials remains questionable.

Acknowledgments. A.A. thanks M.Fabrizio, M.Schirò and C.Aron for useful discussions. A.A. and G.K. have been supported by NSF-DMR-0906943. C.W. was supported by the Swiss Foundation for Science (SNFS). M.C. and A.A. acknowledge financial support from the European Research Council under FP7 Starting Independent Research Grant n.240524 “SUPERBAD”.

-
- [1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (Jan 1996)
 - [2] J. K. Freericks, V. M. Turkowski, and V. Zlatić, *Phys. Rev. Lett.* **97**, 266408 (Dec 2006)
 - [3] P. Schmidt and H. Monien, Arxiv cond-mat/0202046(2002)

- [4] M. Eckstein, M. Kollar, and P. Werner, *Phys. Rev. Lett.* **103**, 056403 (2009) *Phys. Rev. B* **81**, 115131 (2010)
- [5] A. V. Jura, J. K. Freericks, and T. Pruschke, *Phys. Rev. Lett.* **101**, 196401 (2008) J. K. Freericks, *Phys. Rev. B* **77**, 075109 (2008) V. Turkowski and J. K. Freericks, **71**, 085104 (2005)
- [6] M. Eckstein and P. Werner, *Phys. Rev. Lett.* **107**, 186406 (Oct 2011)
- [7] M. Eckstein, T. Oka, and P. Werner, *Phys. Rev. Lett.* **105**, 146404 (2010)
- [8] N. Tsuji, T. Oka, and H. Aoki, *Phys. Rev. Lett.* **103**, 047403 (2009)
- [9] G. Gallavotti, *Statistical Mechanics: a short treatise* (Springer-Verlag, 1999) A. Amaricci, F. Bonetto, and P. Falco, *J. of Math. Phys.* **48**, 072701 (2007)
- [10] G. Gallavotti, Arxiv cond-mat/0701124(2007)
- [11] L. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W.A. Benjamin, Inc., New York, 1962) L. Keldysh, *J. Exp. Theor. Phys.* **47**, 1515 (1964) P. Danielewicz, *Annals of Physics* **152**, 239 (1984)
- [12] The interaction quench is instead expected to influence the dynamics when the coupling to the bath vanishes.
- [13] D. Langreth, *Linear and Non-Linear Transport in Solids* (Plenum Press, New York, 1976)
- [14] H.S.Kohler, N.H.Kwong, and H. A. Yousif, *Comp. Phys. Comm.* **123**, 123 (1999)
- [15] M. Mierzejewski, L. Vidmar, J. Bonča, and P. Prelovšek, *Phys. Rev. Lett.* **106**, 196401 (May 2011)
- [16] C. Aron, C. Weber, and G. Kotliar, Arxiv cond-mat/1105.5387v1(2011)
- [17] A. Polkovnikov, *Annals Phys.* **326**, 486 (2011)